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Summer Internship Project: Set Topology Title:

Author(s): Delan, Mehson Mason

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Summer Internship Project: Set Topology

Mehson Mason Delan

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Presentation Agenda

Goals of Set Topology	Motivation for Set Topology Work	Examples of Set Topology & Use Cases	Future of Set Topology
- Why is it so important to FleCSI?	- It's original ideas and how it can be used.	- Practical physics applications in which we want to utilize it.	- What the foreseeable future holds for this project



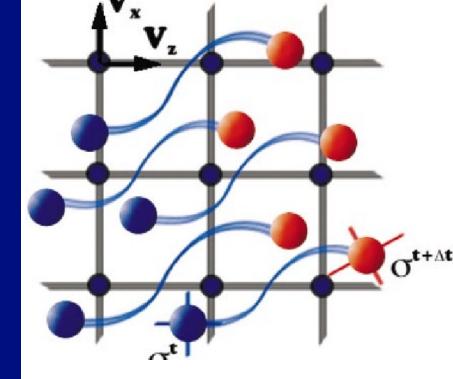
Why a Set Topology?

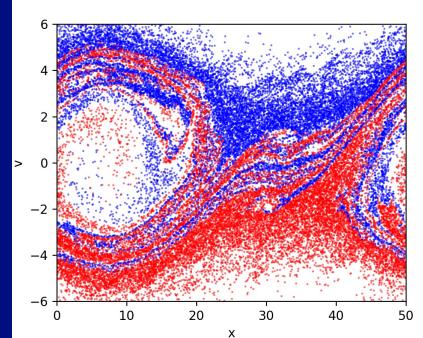
- 1. Expand the array of tools given to physicists, educators, and students.
- 2. Through usages of PIC, MPM, and Monte Carlo.
- 3. My work at LANL was specified to handle requirements for the usage of MPM with FleCSL
- 4. What we want it to do phase change, simulating plasma, and other Multiphysics applications.
- 5. In FleCSI we already have mesh structures, we needed a way to represent those particles and certain behavior's of these particles that clients desire.



Particle-In-Cell Method

- In this method, individual particles (or fluid elements) in a <u>Lagrangian</u> frame are tracked in continuous <u>phase space</u>, whereas moments of the distribution such as densities and currents are computed simultaneously on Eulerian (stationary) <u>mesh</u> points.
- Technique commonly used to simulate motion of charged particles, or plasma.
- Particles do not interact with each other.

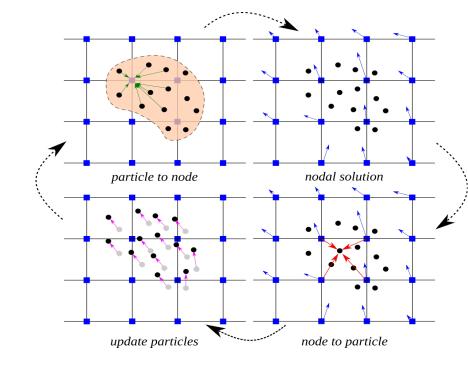


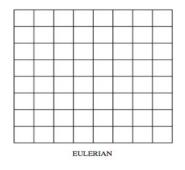


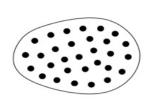


Material Point Method

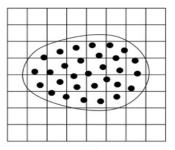
- The need to accurately simulate multimaterial flows and deformations
- drives the development of material point methods (MPMs).
- MPM is a method to solve partial differential equations (PDEs). It is a continuum based method.
- Tracking ejecta from an explosion is a more practical use of this method.







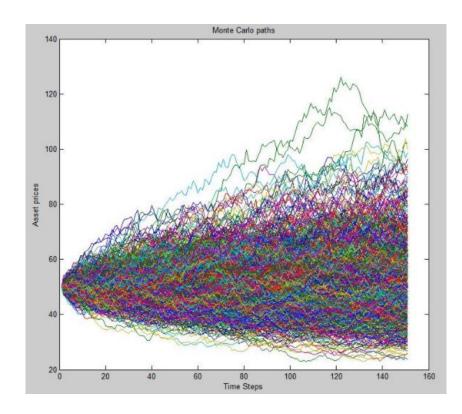
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Monte Carlo

- This method has a large amount of particles that does not have field equations.
- The particles don't interact with each other, they interact with the field.
- Each time you advance the particle you roll a dice and some action takes place to affect the particle (direction, no motion, loses energy, collides with another particle which Changes its energy and direction).





How Set Topology Addresses these Applications

- In both cases (PIC and MPM) we want set topology, because we want to iterate through the particles.
- Particles need to move around in a distributed memory, as well as moving from one color to another (from one part of the domain to another as they evolve).
- Three different physics applications people care about, set is a general utility to facilitate these applications. It moves data around!
- Set topology is flexible enough that there isn't a trade off, we are trying to good software development with FleCSI to cover all these physics applications.
- We want Data structures abstractions that can be specialized using parameterizations that don't hurt performance.
- Template meta programming almost exclusively utilizes compile time ~ good performance.



My Contributions

Set/Interface.hh

- I was able to create an initial interface for set.
- A unit test was written to assume the basic functionality.
- Here we see that the coloring is a vector and each index of that vector represents a grouping of particles.

```
struct set_base {
32
      using coloring = std::vector<std::size_t>;
34
35
      static std::size_t allocate(const std::vector<std::size_t> & arr,
        const std::size_t & i) {
37
         return arr[i];
38
39
    }; // set_base
    template<typename P>
     struct set : set_base {
45
      template<Privileges Priv>
      struct access {
        template<class F>
50
        void send(F &&) {}
51
52
53
      explicit set(coloring x)
        : part{make_repartitioned<P>(x.size(), make_partial<allocate>(x))} {}
55
56
      Color colors() const {
57
58
         return part.colors():
59
60
      template<typename P::index_space>
      data::region & get_region() {
         return part:
64
65
66
      template<typename P::index_space>
       const data::partition & get_partition(field_id_t) const {
69
         return part;
70
71
       repartitioned part;
74
    template<>
    struct detail::base<set> {
      using type = set_base;
```



My Contributions

Set/Interface.hh – Beginning of the Dependent Topology

- Set needs to be initialized with a pointer to an *underlying* topology (slot) which is expected to implement (in its topology accessor) a function from a spatial position (of some unspecified type) to a color. The set specialization should in turn provide a function to obtain a position from a particle (to prevent the underlying topology from needing to know about the particle type).
- The underlying-topology pointer will have to be type-erased in the coloring (though in a much simpler fashion than the linked illustration).

```
struct set_base {
 struct coloring {
    void* ptr;
   std::vector<std::size_t>counts;
 static std::size t allocate(const std::vector<std::size t> & arr,
   const std::size t & i) {
   return arr[i];
}; // set_base
```



Future of the Set Topology

- To refine the concepts, once we get the full-desired functionality of Set working it will be used to satisfy the dependent case where it relies on another topology for a particles coloring.
- We will use another data structure for the case where its independent.
- The real goal is to provide tools for people who want to do different kinds of physics simulations like:
 - 1. N-dimensional tree structure
 - 2. KD tree



Thank You – About Me

- This opportunity has helped me learn about research with the combination of physics and computer science principles, which are my two favorite subjects in school.
- I will be continuing my education from community college to the University of California Santa Barbara pursuing a Statistics and Data Science Degree.
- Working at LANL is definitely an interest of mine in the future.



